Re-derivation of Ewald Summation Formula for Triangular Charge Distribution

By Serdar ACIR

Sabancı University, Turkey

Duke University, USA

We will re-derive E.S. formulation for triangular shape charge distribution.

The triangular shape charge distribution is represented by:

$$SI2 = \begin{cases} \dfrac{3\alpha^4}{\pi}\left(\dfrac{1}{\alpha} - |\mathbf{r}|\right) & \text{for } |\mathbf{r}| \leq 1/\alpha \\ 0 & \text{for } |\mathbf{r}| > 1/\alpha \end{cases}$$

This equation represents a spherically symmetric triangular shape charge distribution whose magnitude is zero when the distance from the atomic center is more than $1/\alpha$. The Ewald coefficient parameter is the only parameter that effects the width of the distribution. The magnitude for $|\mathbf{r}| \leq 1/\alpha$ is given as $\frac{3\alpha^4}{\pi}\left(\frac{1}{\alpha} - |\mathbf{r}|\right)$. The reason why the triangular distribution is represented in this form comes from the definition of the direct sum component. At any point where $|\mathbf{r}| > 1/\alpha$, the net direct sum potential due to the point charge and the charge distribution is zero. Therefore, when computing the force or potential at a point, we can neglect, without error, all charges at a distance greater than $r = 1/\alpha$.

To verify the result; potential component is computed by:

$$\phi_d(r) = \frac{1}{4\pi\epsilon_0}\sum_{B=1}^{N} q_B\left(\frac{1}{|r - R_B|} - \frac{1}{|r - R_B|}\int_0^{1/\alpha} (4\pi a^2\gamma(a))da\right) = 0$$

For the Gaussian the integral becomes:

$$\int_0^{1/\alpha}\left(4\pi a^2\frac{3\alpha^4}{\pi}\left(\frac{1}{\alpha} - |\mathbf{r}|\right)\right)da = 1$$

Since the triangular distribution is defined in two different regions ($|\mathbf{r}| \leq 1/\alpha$ and $|r| > 1/\alpha$), we need to derive the potential for these two regions separately. For $|\mathbf{r}| \leq 1/\alpha$

$$\begin{aligned} \phi_\gamma(r) &= \frac{q_B}{4\pi\epsilon_0}\left(\frac{1}{r}\int_0^r\left(4\pi a^2 3\frac{\alpha^4}{\pi}\left(\frac{1}{\alpha} - a\right)\right)da + \int_r^{1/\alpha}\left(4\pi a 3\frac{\alpha^4}{\pi}\left(\frac{1}{\alpha} - a\right)\right)da\right) \\ &= \frac{q_B}{4\pi\epsilon_0}\left(\alpha(2 + r^2\alpha^2(-2 + r\alpha))\right) \end{aligned}$$

To get the force for the direct sum in this region we simply take the partial derivation of the direct sum potential:

$$\frac{q_B}{4\pi\epsilon_0}\left(\partial_r\left(\frac{1}{r}-\left(\alpha(2+r^2\alpha^2(-2+r\alpha))\right)\right)\right)=\frac{q_B}{4\pi\epsilon_0}\left(\frac{-1+r^3\alpha^3(4-3r\alpha)}{r^2}\right)$$

For $|r|>1/\alpha$:

$$\phi_d(r)=\frac{q_B}{4\pi\epsilon_0}\left(\frac{1}{r}\int_0^{1/\alpha}\left(4\pi a^2 3\frac{\alpha^4}{\pi}\left(\frac{1}{\alpha}-a\right)\right)da\right)=\frac{q_B}{4\pi\epsilon_0}\left(\frac{1}{r}\right)$$

And the direct sum force in this region is:

$$\frac{q_B}{4\pi\epsilon_0}\left(\partial_r\left(\frac{1}{r}-\frac{1}{r}\right)\right)=0$$

And the reciprocal sum potential can be found by:

$$\begin{aligned}\phi_r(r)\quad &=\frac{q_B}{4\pi\epsilon_0}\int_0^{1/\alpha}\left(4\pi r^2\frac{3\alpha^4}{\pi}\left(\frac{1}{\alpha}-r\right)\frac{\mathrm{Sin}[2\pi kr]}{2\pi kr}\right)dr\\ &=\frac{q_B}{4\pi\epsilon_0}\left(\frac{3\alpha^3\mathrm{Sin}\left[\frac{k\pi}{\alpha}\right]\left(-k\pi\mathrm{Cos}\left[\frac{k\pi}{\alpha}\right]+\alpha\mathrm{Sin}\left[\frac{k\pi}{\alpha}\right]\right.}{k^4\pi^4}\right)\end{aligned}$$

Comparing the Gaussian and Triangular Charge Distributions

The preference between the Gaussian and the triangular should depend on the acceptable error and computation time.

The minimum error is possibly achieved by the Gaussian distribution. In the existence of a parallel reciprocal sum, if the total consumed time can be decreased to the time consumed by the direct sum then we can expect the triangular to perform better than the Gaussian at small and large cutoffs (in time) and to perform better in the means of both error and time at small cutoffs.